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<p>Abstract</p> <p>This report outlines the goals, approach, and accomplishments for the Stony Brook Cluster Beam program. We have developed the Cluster Beam method for examining the primary chemistry that occurs in high temperature attack on metal or semi-metal surfaces. The method has been applied to boron, aluminum, and carbon combustion chemistry, and we have been able to identify reactions and products, derive thermochemical information, and convert the data to reaction probabilities that can be fed into combustion models.</p> <p>The report also describes construction and initial operation of a new experiment designed to study the energetics and mechanism of strain energy release in strained hydrocarbon fuel molecules.</p>						
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## **Cluster Beam Studies of Metal Combustion Chemistry**

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### **1. Introduction.**

Our work under this contract was primarily directed toward the overall goal of understanding the chemistry that controls combustion of metal and semi-metal particles added to propellants and explosives to increase energy density. The specific goals and accomplishments are outlined below, and are detailed the list of publications given below.

In addition, during the last year of the contract we began working on a new experiment designed to probe the chemistry and energetics of strained hydrocarbons, which are of interest as high energy fuels. The progress on this work is detailed separately below.

### **2. Cluster Beam Studies of Metal Combustion.**

#### **2.1. Problem and Approach.**

A traditional method for increasing the energy density of fuels has been to incorporate metals such as aluminum or semi-metals such as boron as powders. These materials have high volumetric and gravimetric energy densities, and in some cases also have desirable side effects such as increased bubble energy when added to underwater explosives. In this category, boron is especially desirable for air-breathing propulsion because it has extremely high volumetric energy density. There are a number of problems in achieving the full potential of metal-containing fuels, including slow ignition, incomplete combustion, and formation of undesirable products with lower energy releases.

Some of these problems (particularly unwanted products) are controlled mostly by the homogeneous gas-phase chemistry which goes on after the metal fuel is volatilized. The homogeneous chemistry for boron combustion has been reasonably well worked out in the Aerodyne-Princeton modeling program of Brown et al.<sup>1</sup>, and is nicely summarized in their progress reports. On the other hand, control of ignition and combustion rate are mostly due to heterogeneous chemistry that occurs on the surface of the metal particle. Brown et al. also have attempted to include surface reactions in their model, however the results clearly show the need for experimental data on heterogeneous chemistry of boron. Little is known about the reactions

or their rates at the microscopic level required for accurate combustion modeling.

The chemistry involved in heterogeneous oxidation of metals and semi-metals is complicated, with a large number of elementary reactions contributing to the overall oxidation process. Rosner and co-workers<sup>2,3</sup> have developed a flow-reactor technique to study boron gasification, and have reported results on reactions with  $B_2O_3$  and water. These directly give the overall phenomenological rates, but provide little information about the elementary steps that control the gasification process. Not much is known about these elementary reactions, and it is not at all clear what steps constitute chemical bottlenecks, and how it might be possible to bypass them. Trenary and co-workers<sup>4</sup> have begun the first high-quality experiments on reactions of clean boron surfaces. This work is important because it directly measures the elementary surface chemistry, however it is extremely time consuming. So far they have completed a study of the sticking coefficient for oxygen on the (111) face of single crystal  $\beta$ -rhombohedral boron, and found that dissociative chemisorption is inefficient. This is consistent with the results of our earlier Cluster Beam study<sup>5,6</sup>, which further suggests that this low reactivity is due to an activation energy barrier.

Both conventional kinetics and surface science experiments such as these are valuable in attempting to understand heterogeneous combustion. It is clear however, that there is a need for a method to quickly survey heterogeneous reaction rates over a wide temperature range, but which can also probe the elementary chemistry to provide mechanistic insight. We have developed our Cluster Beam method as a partial solution for these problems. The idea is to use small, well-characterized, singly-ionized clusters containing a few to a few hundred metal atoms, as an experimental representation of a real metal surface under chemical attack. Making this substitution has some real advantages in probing the elementary chemistry.

Using mass spectrometry techniques we can control the exact size and composition of the clusters, and also determine the elementary reaction products directly and unambiguously. We can control the collision energy and cluster internal temperature (with our new variable temperature source) and study the chemistry from room temperature up to thousands of degrees Kelvin. The ability to vary collision energy independently allows us to probe reaction mechanisms and to extract thermochemical parameters for the elementary reactions. This data can then be converted to effective surface reaction rates for input to kinetic modeling programs.

This kind of insight into the cross sections, reaction mechanisms, and thermochemistry

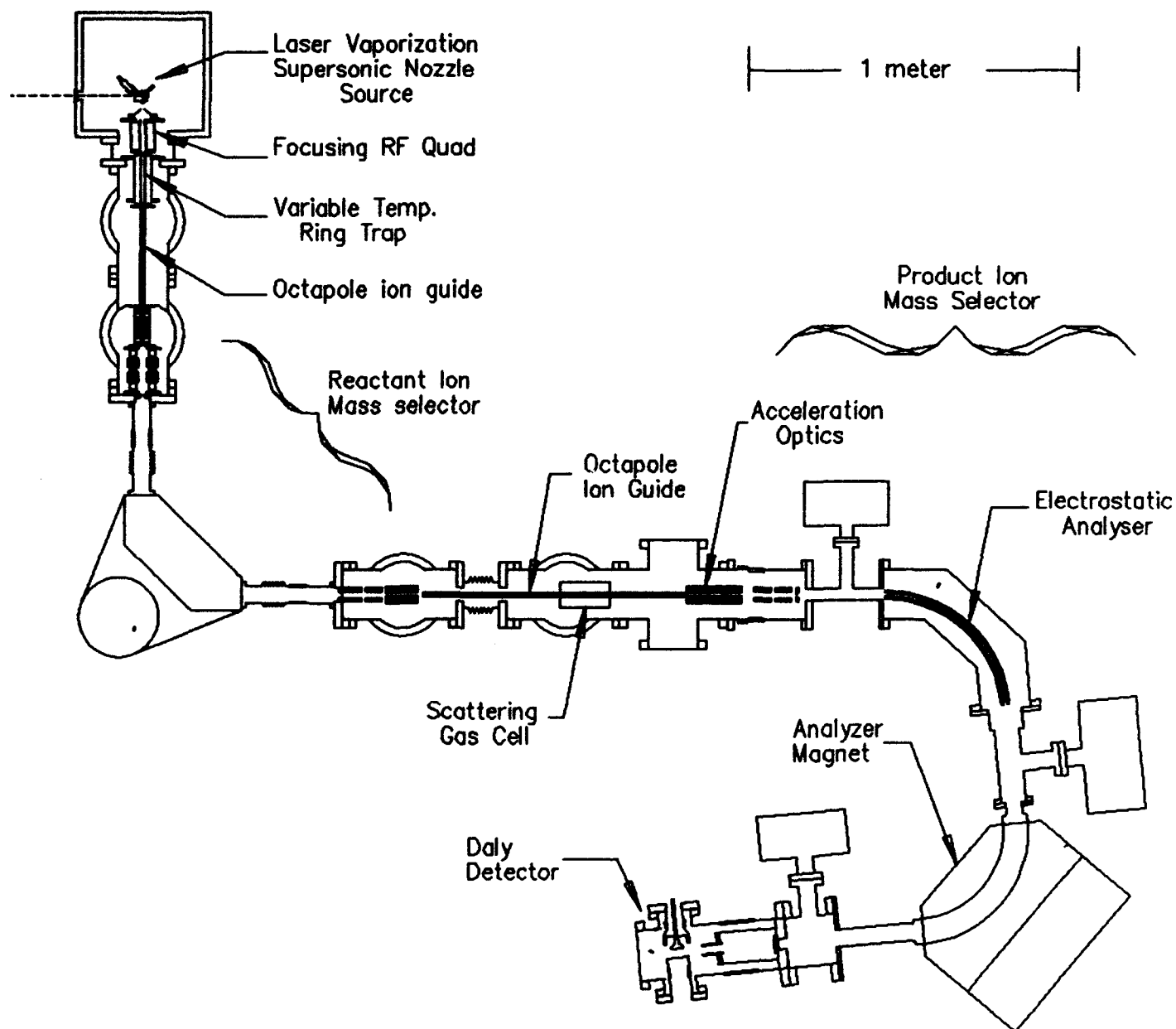
of size and composition selected clusters is of considerable interest in the Cluster Science field as well. Our unique ability to control the internal and collision energies of our cluster reactants has been a real strong point in this aspect of our work. Furthermore, our combustion-motivated work on boron, aluminum, and related simple metal cluster systems has been very timely because we have been able to bring both experimental and theoretical tools to bear.

## 2.2. Results and Current Status.

The results from this contract have been discussed in detail in the 31 publications listed below in section 5. Papers 12 and 14 in that list give comprehensive reviews of our program, and only a short summary is given here.

The major accomplishments to date are:

- Development of cluster ion production and handling techniques for boron, aluminum, carbon, and aluminum-lithium alloys. The techniques can easily be extended to other materials.
- Design and construction of two Cluster Beam tandem, guided-beam, mass spectrometer instruments, each optimized for particular classes of cluster studies. (See Fig. 1 for a schematic diagram of one of the instruments).
- Measurements of reaction cross sections over a wide collision energy range for reaction of boron clusters ( $B_n^+$ ) with  $O_2$ ,  $H_2O$ ,  $CO$ ,  $CO_2$ ,  $H_2$ ,  $CH_4$ ,  $CF_4$ ,  $SiH_4$ ,  $N_2$ ,  $N_2O$ ,  $NO$ ,  $NO_2$ ,  $C_2H_4$ ,  $CH_3OH$ ,  $(CH_3)_2CO$ ,  $NH_3$ ,  $HF$ , and  $CS_2$ .
- Similar studies for reaction of  $Al_n^+$  with  $O_2$ ,  $N_2O$ , and  $H_2O$ .
- Comparative study of  $B_2O_3^+$  reactivity with  $OH$  and  $F$ -containing species such as  $HF/H_2O$ .
- Preliminary study of reactions of  $Al-Li$  alloy clusters with water.
- Conversion of the boron cross section data to surface reaction probabilities for use in combustion models.
- Detailed studies of the reaction mechanisms and thermochemistry for reactions with  $O_2$ ,  $H_2$ ,  $H_2O$ ,  $CO_2$ ,  $N_2O$ , and  $CF_4$ .
- Collision-induced-dissociation studies of boron, carbon, aluminum, aluminum-lithium, and boron oxide cluster ion structures and bonding properties.
- Photodissociation studies of boron and carbon cluster ion structures.
- Soft X-ray absorption spectroscopy of boron and boron rich molecular solids. Measurement of exciton structure near the boron K-edge.
- High level *ab initio* calculation of boron cluster ion structures and properties to compliment



**Figure 1.** Large Stony Brook Cluster Beam Instrument with variable temperature source.

the experimental work.

- Measurements of the effects of cluster isomeric structure on the reactions of carbon cluster ions with  $D_2$ .
- Development of storage techniques for measurement of sequences of chemical reactions.
- Development of pre-reaction techniques to study the bond energies and structures of primary reaction products.
- Development of a new variable temperature cluster source that will allow more accurate simulation of combustion conditions and new fundamental studies of cluster properties.
- Studies of the energy dependence of fullerene interactions with several small atomic and molecular ions. This work capitalized on the unique capabilities of our large Cluster Beam instrument for detailed work on heavy cluster ions.

The boron chemistry results have been used by Brown et al.<sup>1</sup>, in developing their boron combustion model, both to help decide which heterogeneous reactions need to be incorporated into the model, and to estimate rate constants. They also provide insight into the primary mechanisms that control boron volatilization. The instruments that have been developed are general purpose, and should be capable of contributing to understanding many types of high temperature heterogeneous reactions. Currently we are extending our cluster beam work on boron to examine the chemistry with fluorine containing species.

From the cluster science perspective, we have generated a set of benchmark data that is beginning to attract theoretical attention. Currently I am aware of three groups pursuing high level quantum calculations on boron clusters and their chemistry. The synthesis of these calculations and our data should make boron the only cluster system where it is possible to understand in detail the relationships between structure and reactivity. This will be a real breakthrough in the cluster field, and I expect it will attract additional experimental and theoretical work.

### **3. Matrix studies of strained hydrocarbon fuels.**

#### **3.1. Problem and Approach.**

Recent research in chemical synthesis has begun to make strained hydrocarbons a practical

class of high energy fuels<sup>7,8,9,10</sup>. The idea is to produce a synthetic hydrocarbon which has a considerable amount of strain energy incorporated into the molecular framework. These molecules are typically polycyclic, with some or all of the ring systems having highly strained geometries. For example, the cubane isomer of  $C_8H_8$  has a heat of formation ( $\Delta H_f$ ) of about 149 kcal/mole<sup>11</sup>, compared to  $\Delta H_f$  values of 35 to 80 kcal/mole for unstrained  $C_8H_8$  isomers<sup>12</sup>. This means that ~100 kcal/mole of energy is stored in the material, purely in the form of strain. The resulting high energy density is due partly to added strain energy, and partly to increased fuel density (the molecules are more compact than unstrained analogs). In combustion, the volumetric energy density can be increased by up to 60% compared to normal fuels.

Another potential effect of the strain energy is in accelerating and controlling combustion. It may be possible to initiate controlled release of the strain energy while the fuel is still in droplet (or solid) form. This energy release would transform a liquid fuel into a hot vapor on a microsecond time scale. In addition, the isomerization may produce copious free radicals which can initiate and participate in combustion chain reactions. The combination could make these fuels burn much faster than conventional hydrocarbons, which might find application in hypersonic combustion. Of course, uncontrolled strain release could cause serious stability problems, therefore understanding the initiation, evolution, and control of strain release is a key problem in utilizing these fuels.

During the last year of this contract we began developing an experiment to probe the energetics and mechanism of strain release. The basic idea is to isolate candidate molecules in a cryogenic matrix, then photolyze at different photon energies. The effect of photolysis is monitored by a combination of mass spectrometry and *in situ* Fourier-transform infrared spectroscopy. This will allow us to measure the energy required to initiate isomerization, and will also provide information regarding the strain release products. The experiments can be done on isolated molecules, neat samples, or on mixtures.

### 3.2. Results and Current Status.

During the past year we have constructed (using equipment funds provided by the State of New York) the instrument shown in Figs. 2 and 3, which give side and top views respectively. In the side view, the cryo-substrate, which is a gold-coated sapphire block mounted on a 10K closed-cycle helium refrigerator, is shown mounted from the bottom of the main

chamber. Not shown is a low temperature ( $\sim 80\text{K}$ ) shroud that reduces the radiative heat load on the  $10\text{K}$  surface. On the top of the chamber we have a precision x-y-z manipulator on which we mount a  $80\text{K}$  mask to control the exposure area of the sample. Also mounted from the top is the gas inlet system (not shown) which consists of two gas jets directed at the cryo-substrate. Immediately opposite the sample is the mass spectrometer.

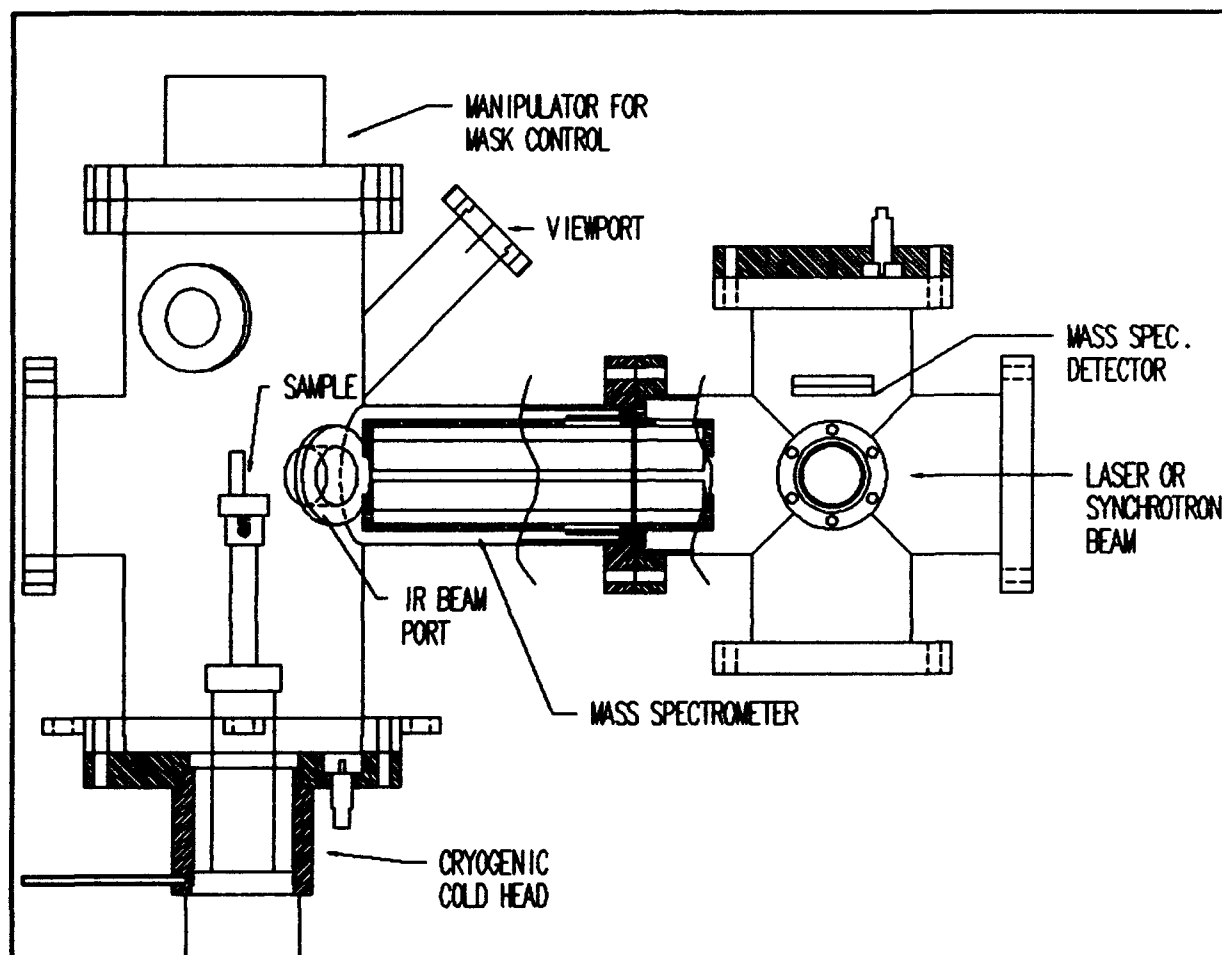


Figure 2. Side view of Matrix Isolation instrument.

Ions desorbing from the sample, or produced by electron impact ionization of neutrals leaving the sample, are accelerated, passed through a quadrupole mass filter, then detected by an off-axis CEMA detector. The aperture of the mass spectrometer is large enough to allow passage of the laser or synchrotron beam. The entire system is UHV compatible and is pumped by a magnetically levitated turbomolecular pump.

The optical layout can be seen more clearly in the top-view shown in Fig. 3. The laser or synchrotron beam passes through the mass filter, then irradiates a spot on the sample. Any material desorbing from the sample can be analyzed simultaneously by the mass spectrometer

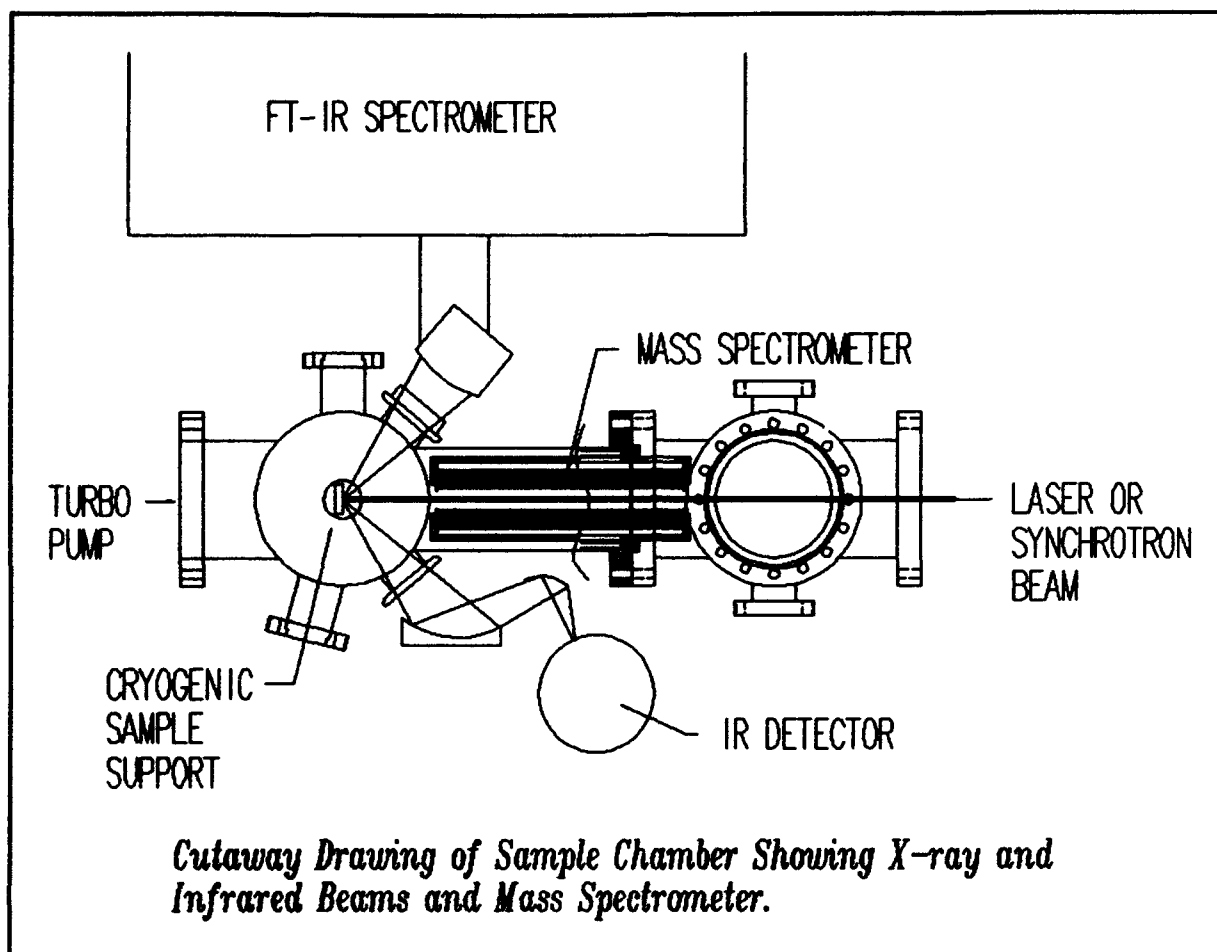


Figure 3. Top view of Matrix Isolation instrument.

system. Infrared spectroscopy is done in reflection mode. A Mattson 5020 FT-IR spectrometer is used to produce a collimated, modulated infrared beam. This is focused onto the cryo-substrate so that it overlaps with the spot irradiated by the laser or synchrotron. The focused beam is reflected by the gold coated substrate, collected by a set of mirrors, and demagnified onto a liquid nitrogen cooled MCT detector. The entire IR beam path is either evacuated or purged to eliminate interference from atmospheric gases.

The entire instrument is complete, including both FT-IR and mass spectrometers. At present, we are lacking a dye laser source for the photolysis experiments, so we have gone ahead with "tune-up" experiments using the U15 beamline at the National Synchrotron Light Source. We have completed two runs at the synchrotron in December-January and March, focusing mainly on checking our experimental method and working out the bugs in the instrument. All in all, the runs were quite productive, and we are analyzing the data for publication.

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2. "Metal Cluster Ion Chemistry", Scott L. Anderson and Luke Hanley, SPIE 669 (1986) 133.
3. "Reactions of Bare Aluminum Cluster Ions", Luke Hanley and Scott L. Anderson, Chem. Phys. Lett. 129 (1986) 429.
4. "Chemistry of Small Metal Cluster Ions", Luke Hanley, Stephen Ruatta, and Scott L. Anderson, in The Physics and Chemistry of Small Clusters, Jena and Rao eds., Plenum, New York (1986).
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8. "Reaction of Aluminum Cluster Ions with Oxygen and Nitrous Oxide: Energetics and Dynamics of Cluster Oxidation", Stephen A. Ruatta, Luke Hanley, and Scott L. Anderson, J. Chem. Phys. 89 (1988) 273.
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11. "Dynamics of Boron Cluster Ion Reactions with Deuterium: Adduct Formation and Decay", Stephen A. Ruatta, Luke Hanley, and Scott L. Anderson, J. Chem. Phys. 91 (1989) 226.
12. "Cluster Based Reaction Probabilities for Boron with Oxygen, Hydrogen, Water, Nitrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide, Methane, Tetrafluoromethane, and Silane", P. A. Hintz, S. A. Ruatta, and S. L. Anderson, Tech. Report #SBIL-A89, submitted to DTIS, 1989, Oct. 28.
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17. "Chemistry With Cluster Ions", Scott L. Anderson, in Clusters of Atoms and Molecules, H. Haberland, ed. Springer, Heidelberg, (in press).
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26. "Chemistry of Metal and Semi-Metal Cluster Ions", Denise C. Parent and Scott L. Anderson, Chem. Rev. (submitted 5/92).
27. " $O^+ + C_{60}$ :  $C_{60}O^+$  Production and Decomposition, Charge Transfer, and Formation of  $C_{59}O^+$ : Dopeyball or  $[CO@C_{58}]^+$ ", James F. Christian, Zhimin Wan, and Scott L. Anderson, Chem. Phys. Lett. (submitted 6/92)
28. "Oxidation of Small Carbon Cluster Ions by  $O_2$ : Effects of Structure on the Reaction Mechanism", Marianne B. Sowa and Scott L. Anderson, J. Chem. Phys. (submitted).

**5.2. Publications in preparation resulting from work completed during this contract.**

29. "A Comparison of Boron Cluster Ion Reactivity with  $CO$ ,  $CH_4$ ,  $CF_4$ ,  $SiH_4$ ,  $C_2H_4$ ,  $CH_3OH$ ,  $(CH_3)_2CO$ , and  $NH_3$ ", Paul A. Hintz, Marianne B. Sowa, Stephen A. Ruatta, and Scott L. Anderson, (in preparation for J. Phys. Chem.).
30. "A Triple Sector Guided-Beam Mass Spectrometer for Beam Studies of Large Cluster Ions", James M. Christian, Zhimin Wan, and Scott L. Anderson, (in preparation for Rev. Sci. Instrum.).
31. "Boron K-Edge Spectra of Solid Boron,  $B_4C$ ,  $BN$ , and  $o-B_{10}C_2H_{12}$ ", Scott L. Anderson, Kazuyuki Tohji, and Yasuo Udagawa, (in preparation).

**5.3. Number of significant presentations Total: 50 (broken down by category):**

- a. Invited lectures at scientific meetings: 9 (not including contractor's meetings)
- b. Invited lectures at US universities or corporations: 15
- c. Invited lectures at foreign universities: 5
- d. Contributed papers at scientific meetings: 21